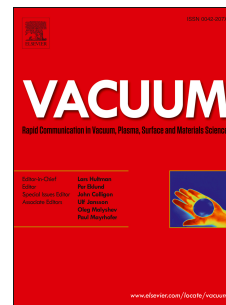


# Accepted Manuscript

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PII: S0042-207X(16)30279-2

DOI: [10.1016/j.vacuum.2016.11.025](https://doi.org/10.1016/j.vacuum.2016.11.025)

Reference: VAC 7207

To appear in: *Vacuum*

Received Date: 19 July 2016

Revised Date: 22 October 2016

Accepted Date: 16 November 2016

Please cite this article as: Izakmehri Z, Ganji MD, Ardjmand M, Adsorption of 2, 3, 7, 8-tetrachlorodibenzo-p-dioxin (TCDD) on pristine, defected and Al-doped carbon nanotube: A dispersion corrected DFT study, *Vacuum* (2016), doi: 10.1016/j.vacuum.2016.11.025.

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# Adsorption of 2, 3, 7, 8-Tetrachlorodibenzo-p-dioxin (TCDD) on pristine, defected and Al-doped carbon nanotube: A dispersion corrected DFT study

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## Abstract:

The effective enrichment and detection of organic pollutants in the environment has been attracted much attention because of enormous concerns about human health. Using dispersion-corrected density functional theory (DFT-D2), the interactions between 2, 3, 7, 8-tetrachlorodibenzo-p-dioxin (TCDD) and pristine, defected and Al-doped carbon nanotubes (Al-CNT) were studied. The TCDD molecule was physisorbed on a pure CNT and CNT contain defects with binding energies of about -0.52 eV and -0.34 eV, respectively. The accuracy of our method was validated by hybrid B3LYP levels of theory and it was shown that there is a worthy agreement between two respected methods. However, the binding energy rises to -0.85 eV when TCDD binds to Al-CNT. The increase in binding energy is due to charge transfer from the

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